

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
 Data File : VX031552.D
 Acq On : 22 Sep 2022 06:06
 Operator : JC/MD
 Sample : N4642-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 46 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-6R

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
 Title : SW846 8260

Signal : TIC: VX031552.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.391	694	706	719	rBV	80554	229133	10.59%	1.225%
2	5.556	719	733	756	rVB2	77944	233308	10.79%	1.248%
3	5.958	789	799	813	rBV2	88839	231723	10.71%	1.239%
4	6.763	922	931	945	rBV	117759	281528	13.02%	1.505%
5	7.379	1022	1032	1042	rVB3	13379	33737	1.56%	0.180%
6	8.427	1198	1204	1210	rBV2	18998	34032	1.57%	0.182%
7	8.647	1235	1240	1247	rVB	433116	678679	31.38%	3.629%
8	8.720	1247	1252	1258	rBV	96912	143026	6.61%	0.765%
9	8.958	1281	1291	1300	rBV	103697	171138	7.91%	0.915%
10	9.049	1300	1306	1311	rBV	127106	187012	8.65%	1.000%
11	9.458	1365	1373	1377	rBV3	13767	23591	1.09%	0.126%
12	10.055	1462	1471	1477	rBV	268504	363865	16.82%	1.946%
13	10.195	1488	1494	1500	rBV	937431	1183685	54.72%	6.329%
14	10.305	1505	1512	1519	rVB	1085598	1332793	61.62%	7.127%
15	10.640	1562	1567	1574	rVB	341317	448219	20.72%	2.397%
16	10.963	1614	1620	1625	rVB	108736	133752	6.18%	0.715%
17	11.079	1634	1639	1645	rBV	384383	493278	22.81%	2.638%
18	11.305	1668	1676	1681	rBV	222358	274212	12.68%	1.466%
19	11.378	1683	1688	1696	rVV	530385	961432	44.45%	5.141%
20	11.451	1696	1700	1710	rVB	448235	544909	25.19%	2.914%
21	11.616	1721	1727	1737	rBV	882560	1081668	50.01%	5.784%
22	11.756	1744	1750	1755	rBV	1867772	2162985	100.00%	11.566%
23	11.890	1770	1772	1780	rVB	18214	21970	1.02%	0.117%
24	11.969	1780	1785	1789	rBV	27696	36622	1.69%	0.196%
25	12.024	1789	1794	1799	rVB	329215	415468	19.21%	2.222%
26	12.091	1799	1805	1810	rBV	997494	1238895	57.28%	6.624%
27	12.244	1824	1830	1838	rBV	876583	1130115	52.25%	6.043%
28	12.317	1838	1842	1849	rVB3	135632	201591	9.32%	1.078%
29	12.414	1850	1858	1862	rBV2	59684	86420	4.00%	0.462%
30	12.463	1862	1866	1871	rVB	67802	78101	3.61%	0.418%
31	12.530	1873	1877	1879	rBV	101239	119409	5.52%	0.638%
32	12.555	1879	1881	1886	rVB	70047	78809	3.64%	0.421%
33	12.615	1886	1891	1894	rBV	166008	200541	9.27%	1.072%
34	12.646	1894	1896	1900	rVB	60775	61932	2.86%	0.331%
35	12.701	1900	1905	1913	rBV2	235007	316420	14.63%	1.692%
36	12.847	1925	1929	1935	rVB	73451	93354	4.32%	0.499%

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Integration Parameters: RTEINT.P

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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37	12.920	1935	1941	1945	rBV	165878	213522	9.87%	1.142%
38	12.963	1945	1948	1953	rVB	150645	175728	8.12%	0.940%
39	13.036	1953	1960	1964	rBV6	11124	26812	1.24%	0.143%
40	13.170	1978	1982	1986	rVB	153749	181253	8.38%	0.969%
41	13.292	1997	2002	2007	rVB2	459119	589619	27.26%	3.153%
42	13.347	2007	2011	2014	rBV3	23002	30113	1.39%	0.161%
43	13.426	2019	2024	2031	rVB	71880	99551	4.60%	0.532%
44	13.506	2031	2037	2040	rBV2	16414	22084	1.02%	0.118%
45	13.548	2040	2044	2046	rBV	30585	39885	1.84%	0.213%
46	13.585	2046	2050	2055	rVB3	35259	51400	2.38%	0.275%
47	13.664	2060	2063	2068	rVB2	44009	58744	2.72%	0.314%
48	13.774	2076	2081	2088	rVV	1048859	1311283	60.62%	7.012%
49	13.871	2088	2097	2102	rVB	85210	121795	5.63%	0.651%
50	14.079	2126	2131	2135	rBV	18690	24434	1.13%	0.131%
51	14.213	2150	2153	2159	rVB	21412	30300	1.40%	0.162%
52	14.597	2211	2216	2219	rBV	33958	43198	2.00%	0.231%
53	14.640	2219	2223	2234	rVB	172178	222251	10.28%	1.188%
54	14.780	2241	2246	2255	rVB2	115327	152535	7.05%	0.816%

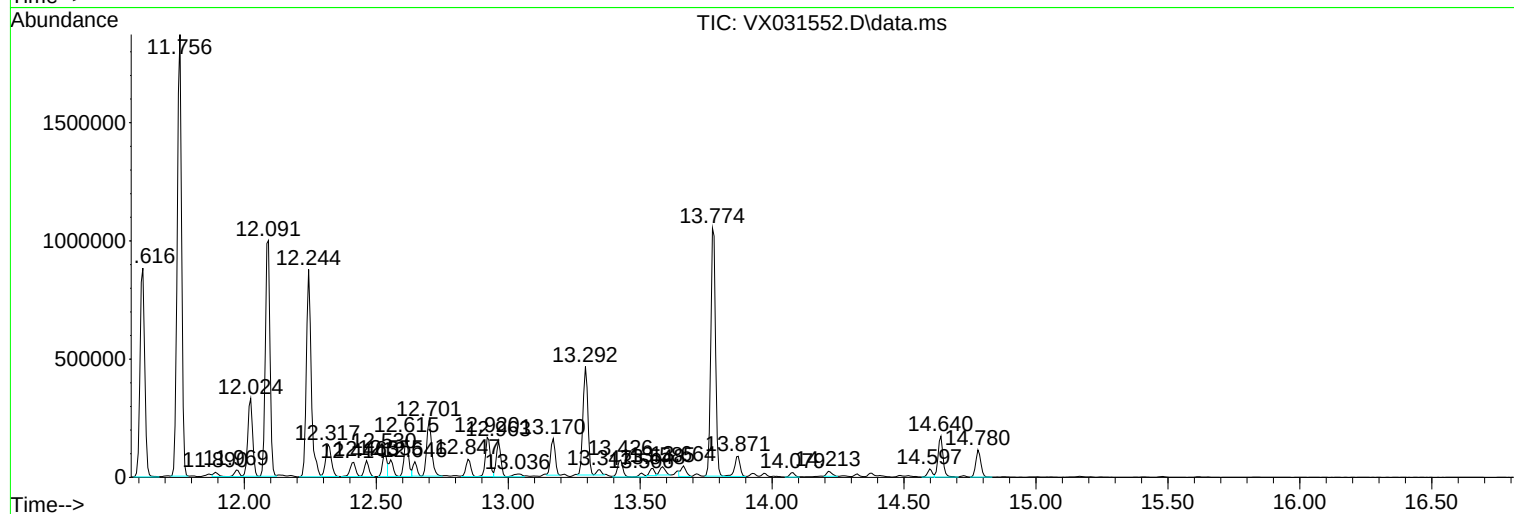
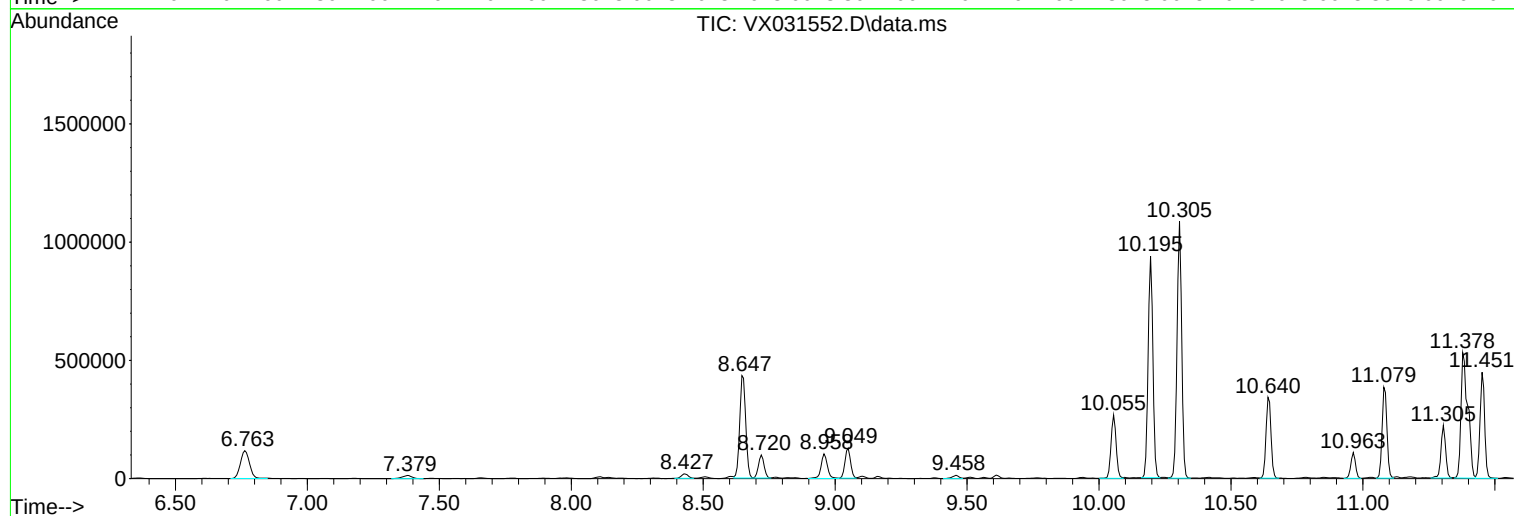
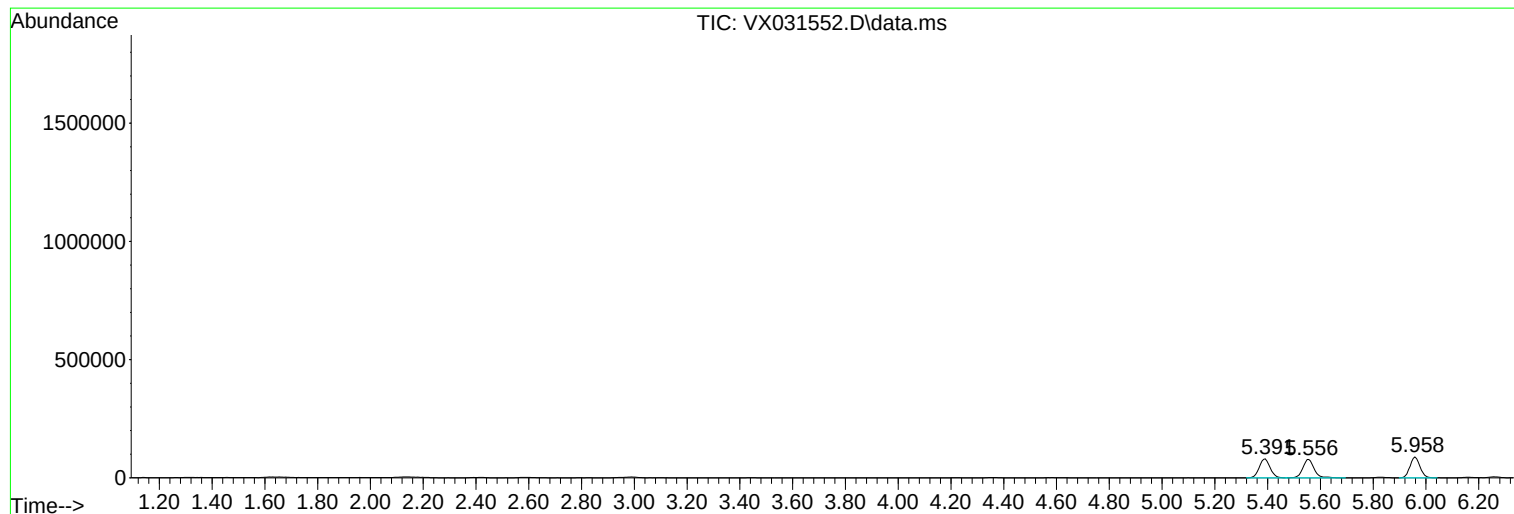
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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Instrument :
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ClientSampleId :
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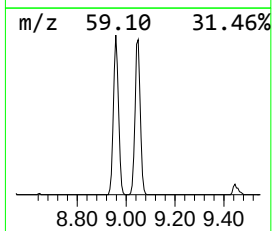
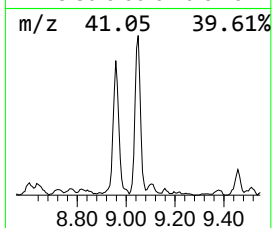
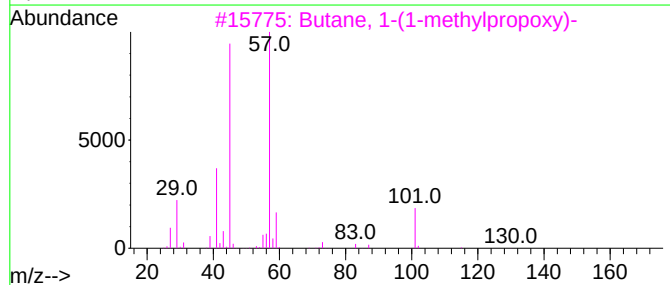
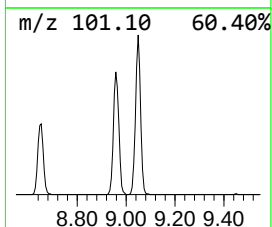
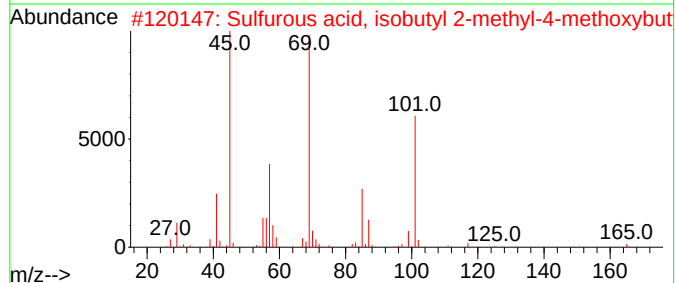
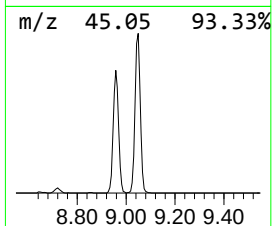
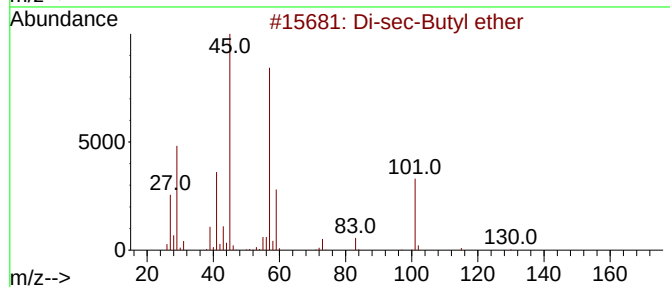
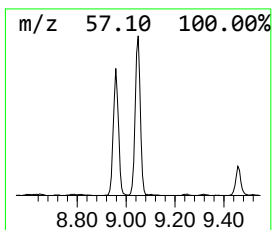
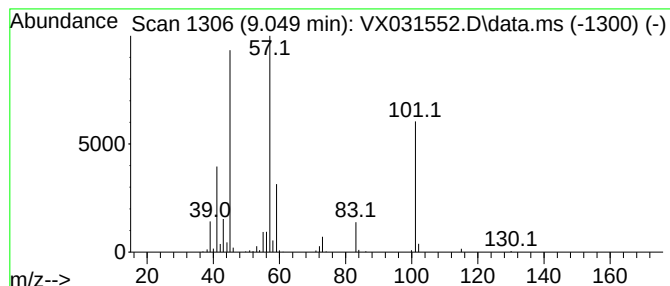
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Di-sec-Butyl ether Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.049	25.70 ug/l	187012	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Di-sec-Butyl ether	130	C8H18O	006863-58-7	91
2			Sulfurous acid, isobutyl 2-methy...	238	C10H22O4S	1000309-20-3	59
3			Butane, 1-(1-methylpropoxy)-	130	C8H18O	000999-65-5	53
4			Sulfurous acid, di(2-methyl-4-me...	282	C12H26O5S	1000309-20-7	50
5			2-t-Butyl-5-methyl[1,3]dioxolan...	158	C8H14O3	130930-47-1	39



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ALS Vial : 46 Sample Multiplier: 1

Instrument :
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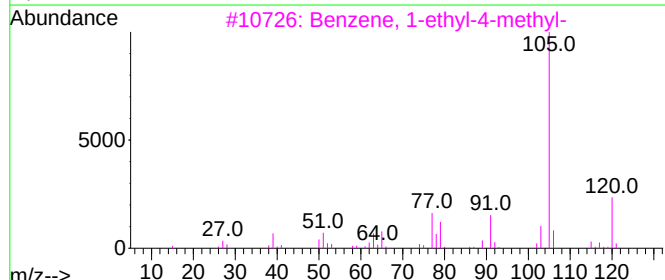
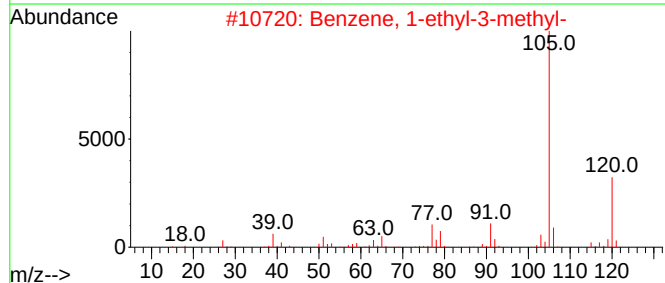
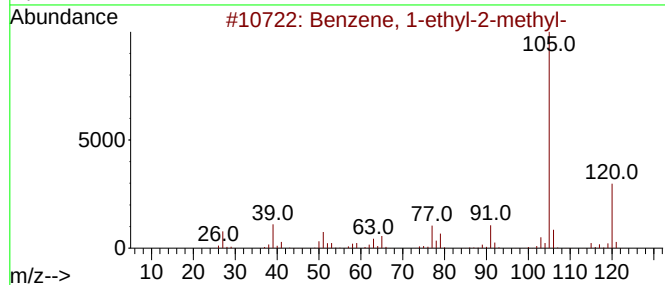
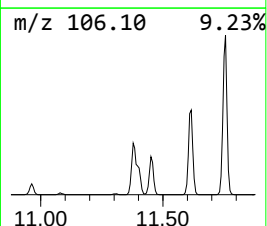
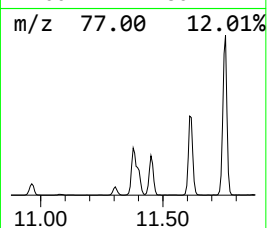
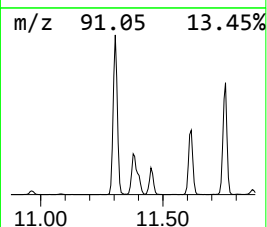
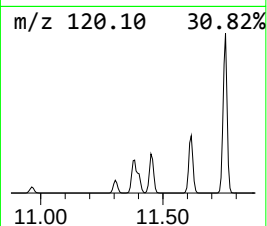
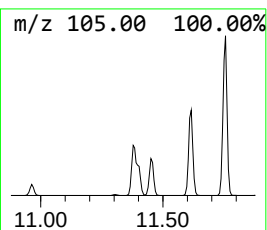
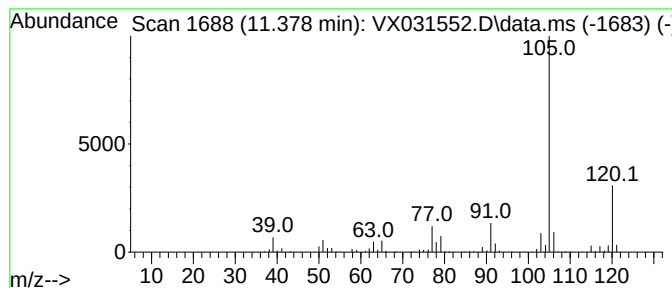
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.378	115.71 ug/l	961432	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	95
2			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	95
3			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
5			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
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Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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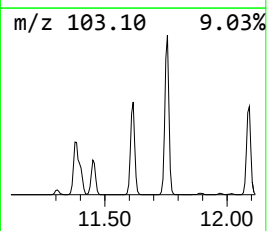
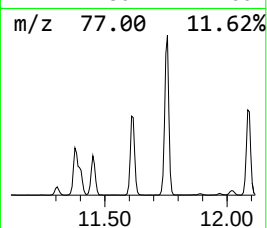
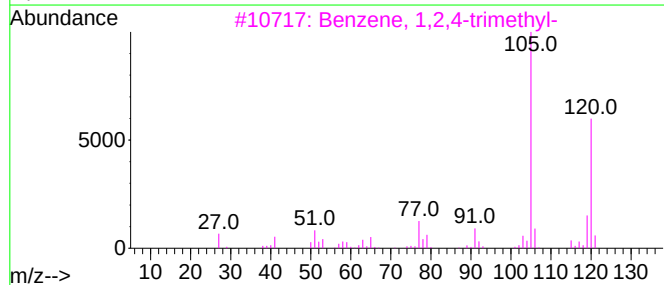
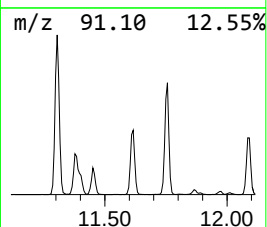
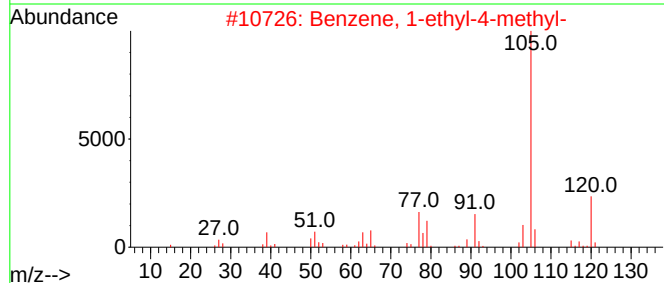
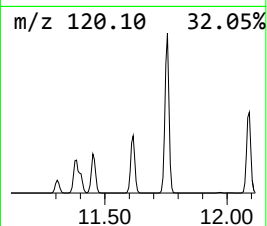
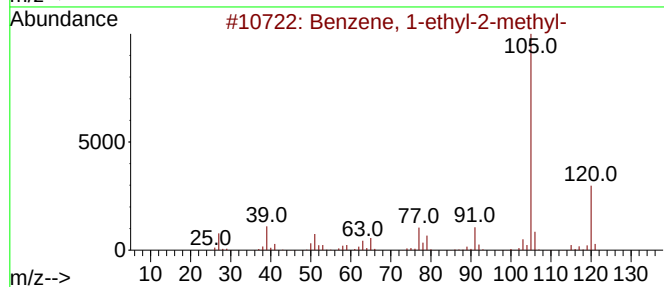
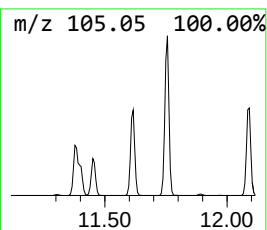
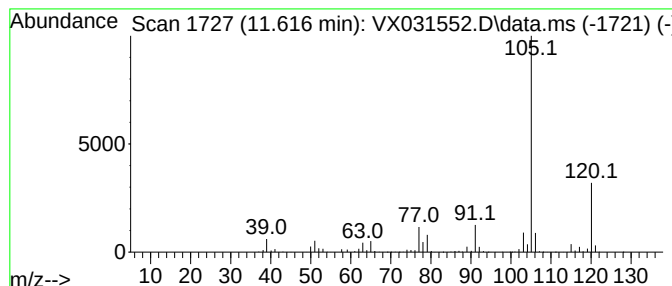
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Benzene, 1-ethyl-4-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.616	130.18 ug/l	1081670	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	94
2			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	93
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	91
5			Mesitylene	120	C9H12	000108-67-8	91



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Instrument :
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ClientSampleId :
MW-6R

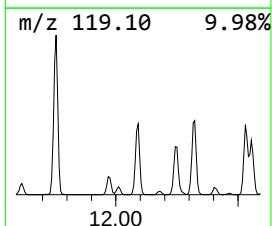
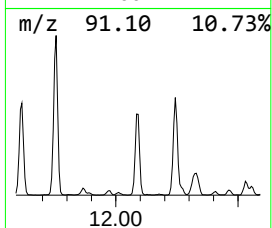
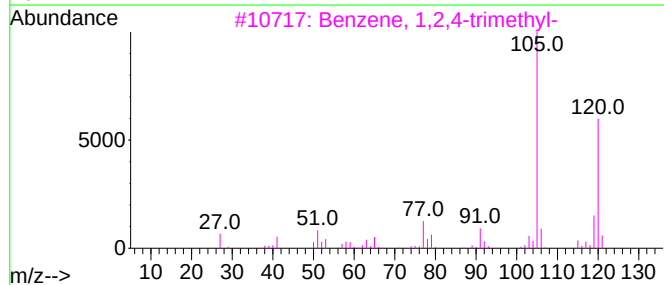
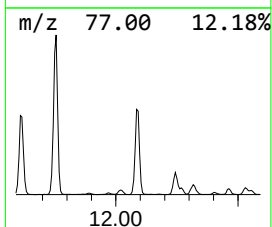
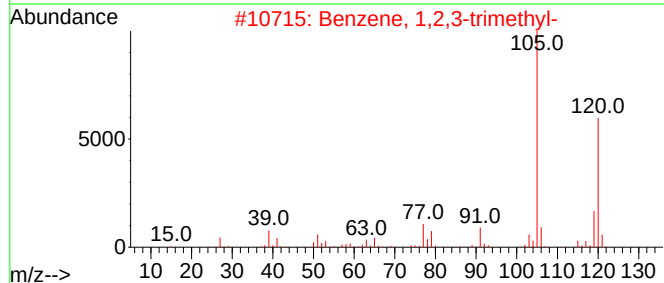
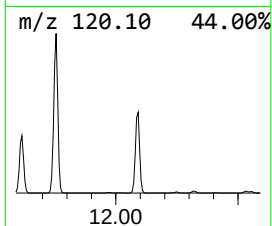
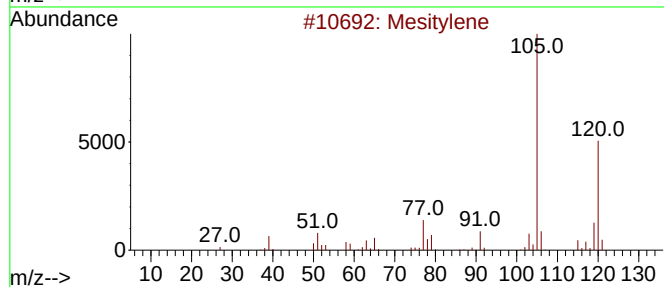
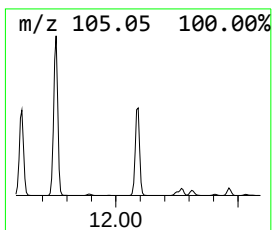
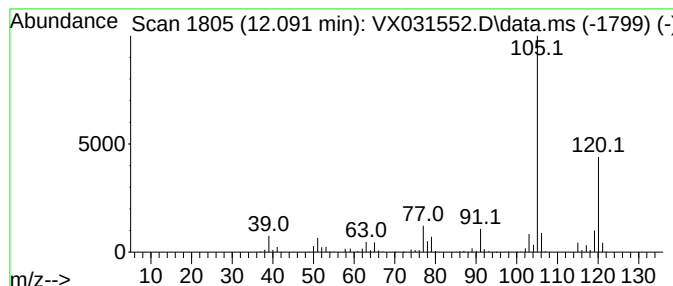
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1,2,3-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.091	149.10 ug/l	1238900	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Mesitylene	120	C9H12	000108-67-8	97
2			Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	95
3			Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	91
4			Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91
5			Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	90



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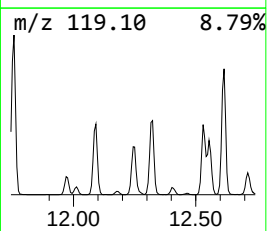
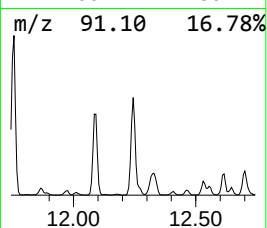
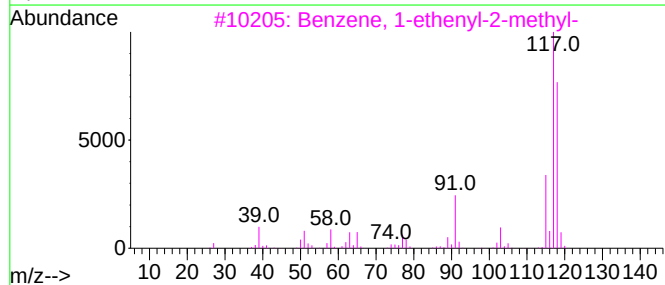
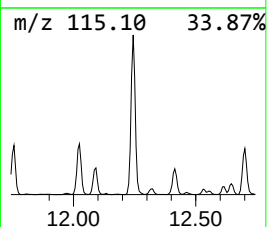
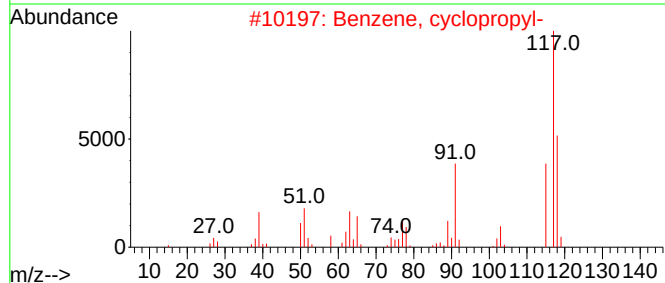
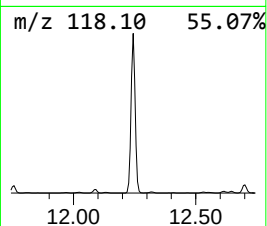
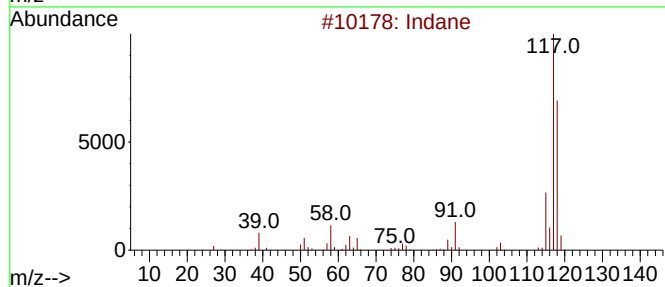
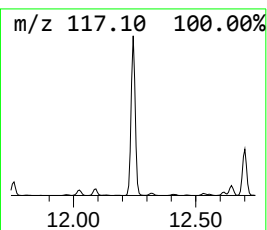
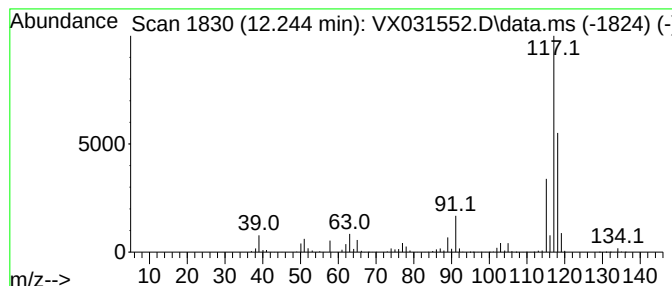
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Indane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.244	136.01 ug/l	1130120	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Indane	118	C9H10	000496-11-7	87
2			Benzene, cyclopropyl-	118	C9H10	000873-49-4	81
3			Benzene, 1-ethenyl-2-methyl-	118	C9H10	000611-15-4	81
4			Benzene, 2-propenyl-	118	C9H10	000300-57-2	74
5			Deltacyclene	118	C9H10	007785-10-6	68



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

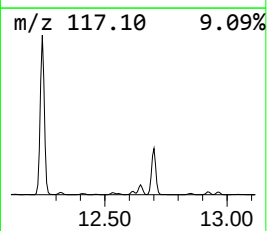
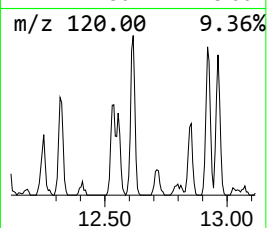
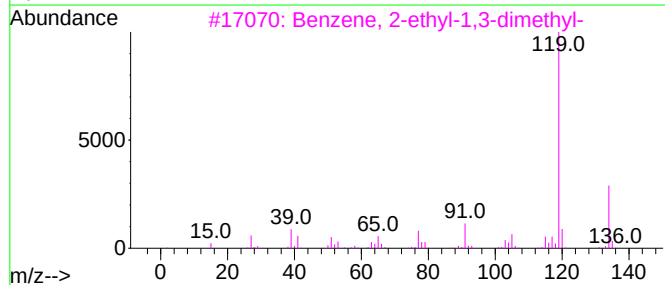
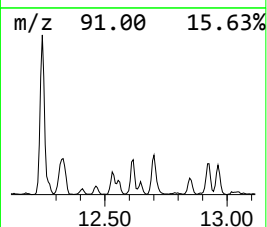
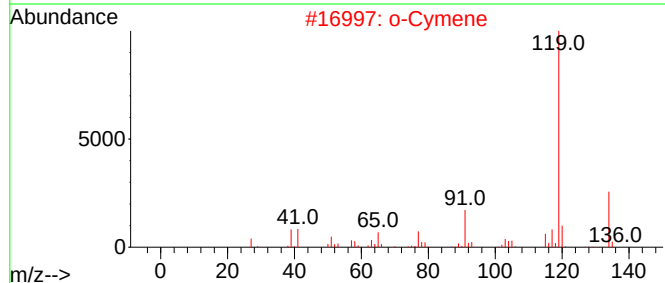
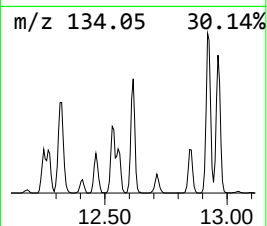
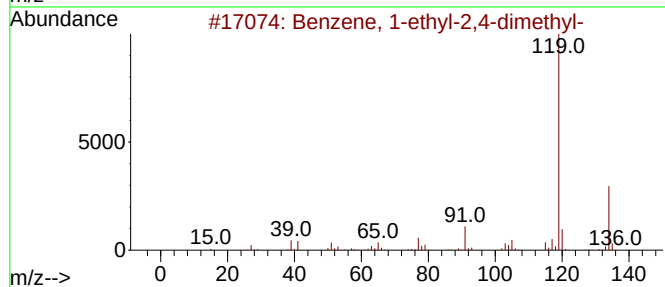
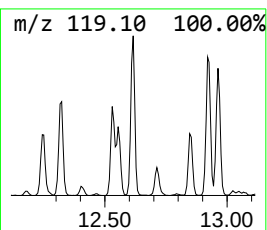
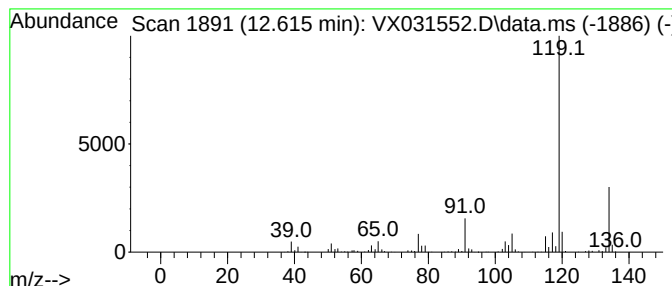
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzene, 1-ethyl-2,4-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.616	24.13 ug/l	200541	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	97
2			o-Cymene	134	C10H14	000527-84-4	97
3			Benzene, 2-ethyl-1,3-dimethyl-	134	C10H14	002870-04-4	95
4			Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	94
5			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	94



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

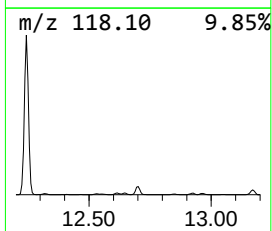
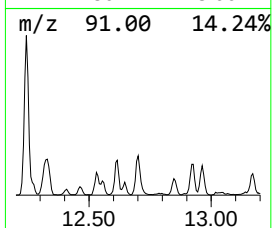
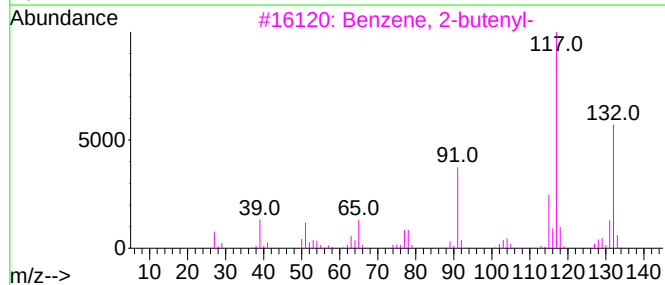
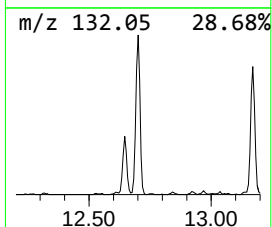
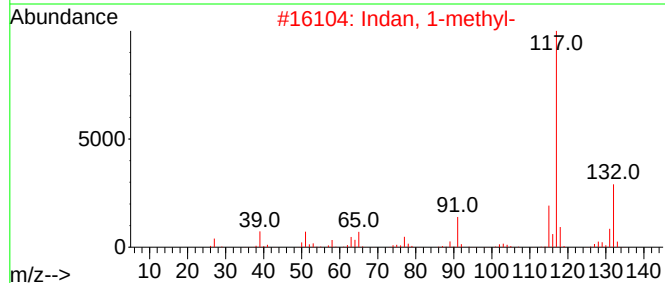
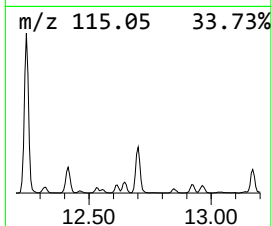
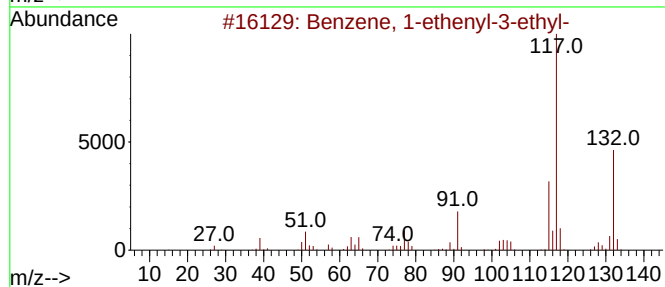
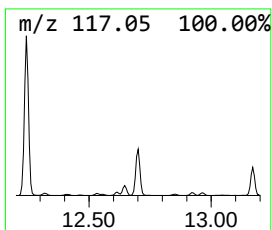
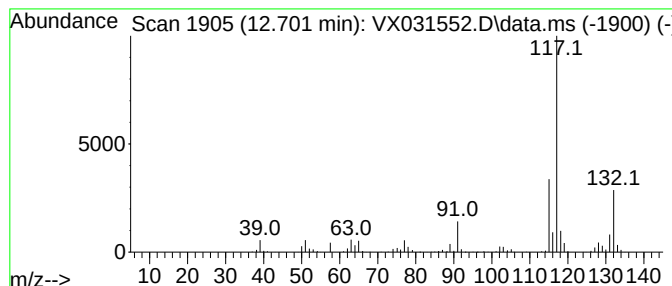
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Benzene, 1-ethenyl-3-ethyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.701	38.08 ug/l	316420	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-ethenyl-3-ethyl-	132	C10H12	007525-62-4	91
2			Indan, 1-methyl-	132	C10H12	000767-58-8	87
3			Benzene, 2-butenyl-	132	C10H12	001560-06-1	83
4			1-Methyl-2-phenylcyclopropane	132	C10H12	003145-76-4	83
5			Benzene, (2-methyl-2-propenyl)-	132	C10H12	003290-53-7	80



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

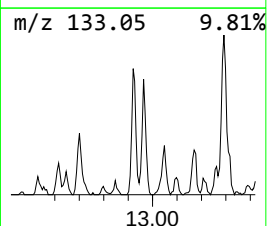
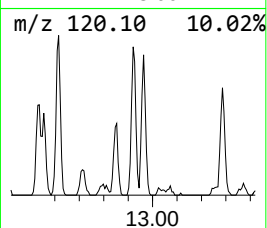
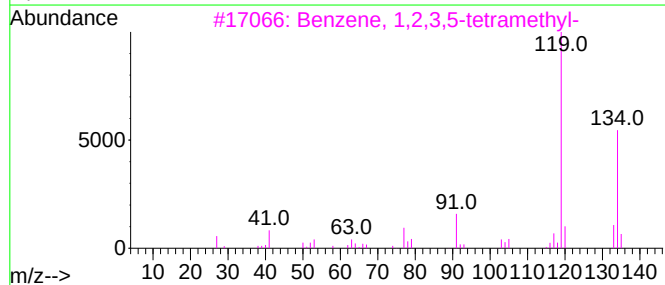
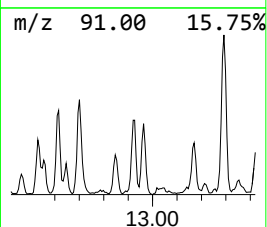
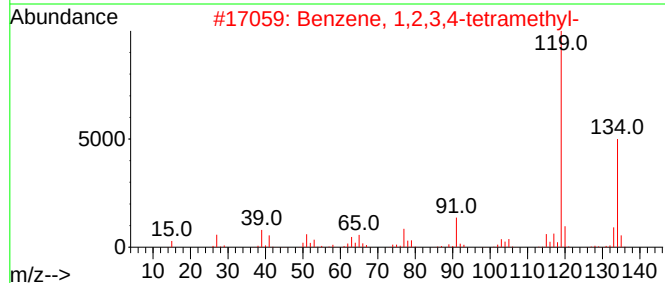
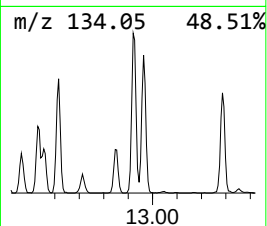
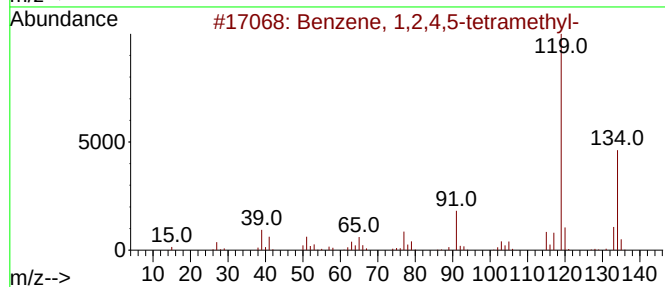
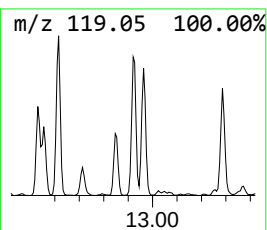
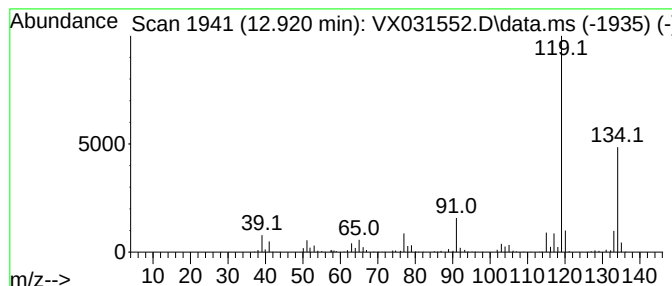
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 Benzene, 1,2,4,5-tetramethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.920	25.70 ug/l	213522	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1,2,4,5-tetramethyl-	134	C10H14	000095-93-2	97
2			Benzene, 1,2,3,4-tetramethyl-	134	C10H14	000488-23-3	97
3			Benzene, 1,2,3,5-tetramethyl-	134	C10H14	000527-53-7	96
4			o-Cymene	134	C10H14	000527-84-4	93
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	93



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

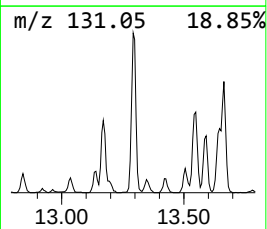
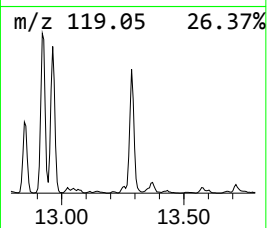
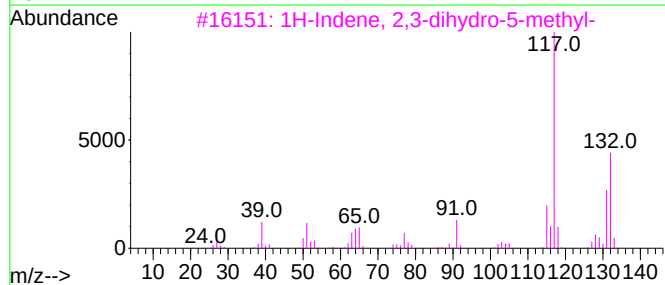
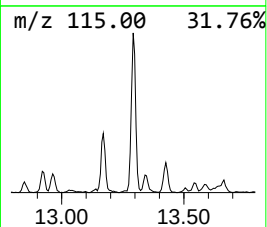
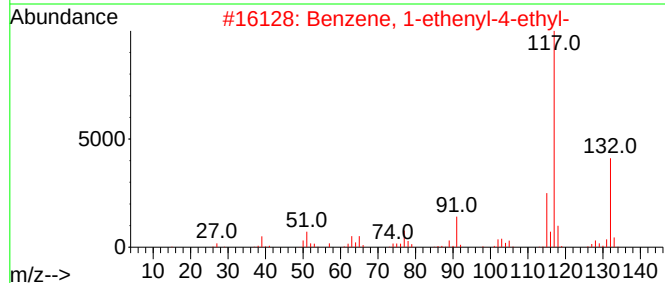
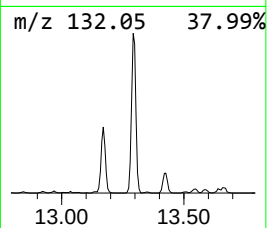
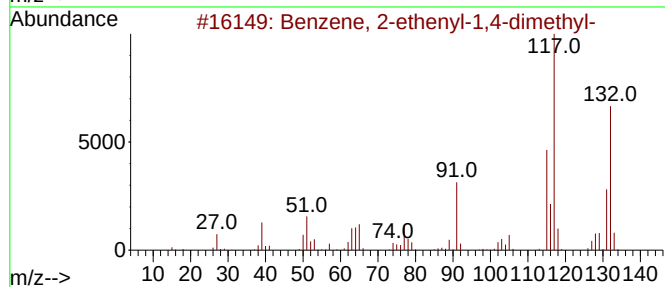
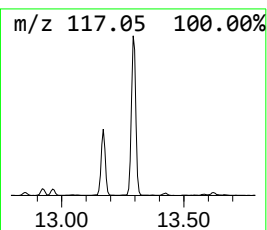
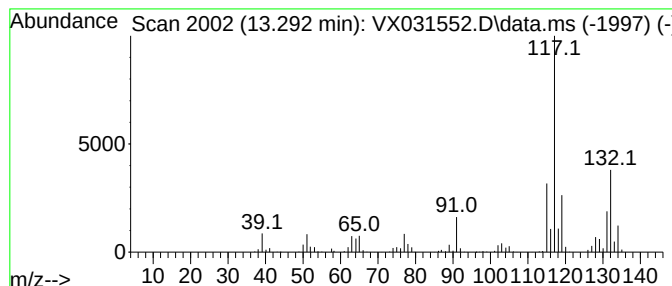
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzene, 2-ethenyl-1,4-dime... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.292	70.96 ug/l	589619	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 2-ethenyl-1,4-dimethyl-	132	C10H12	002039-89-6	95
2			Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	94
3			1H-Indene, 2,3-dihydro-5-methyl-	132	C10H12	000874-35-1	94
4			1H-Indene, 2,3-dihydro-4-methyl-	132	C10H12	000824-22-6	93
5			1-Phenyl-1-butene	132	C10H12	000824-90-8	91



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

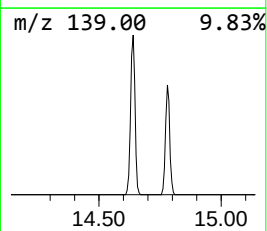
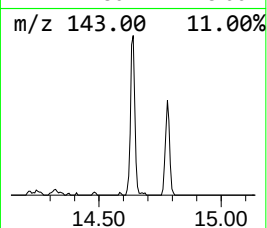
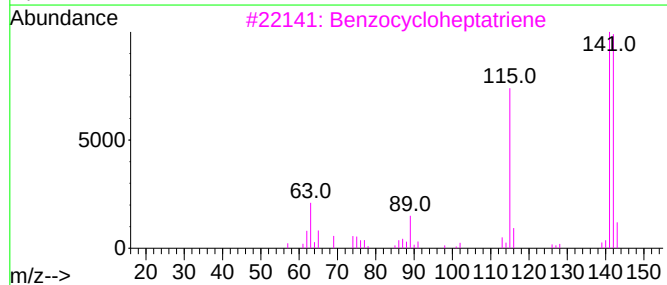
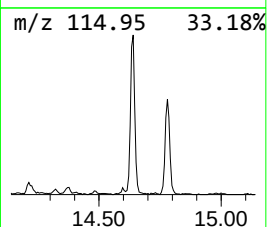
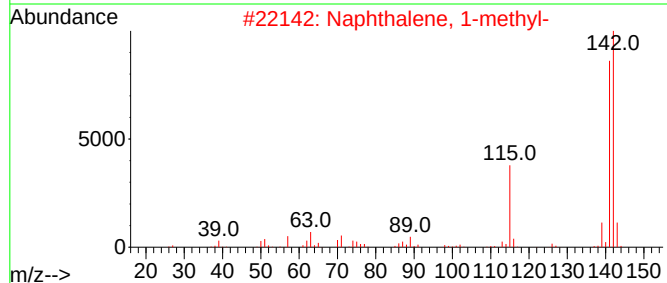
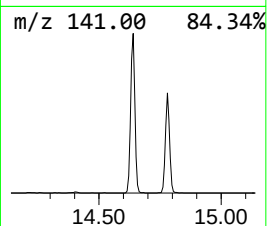
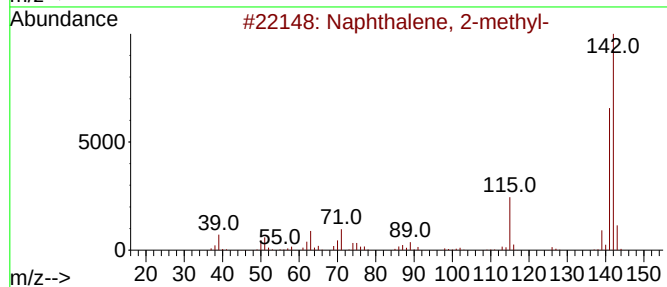
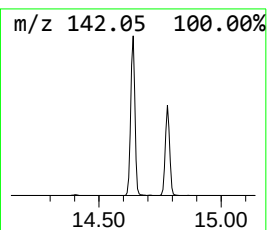
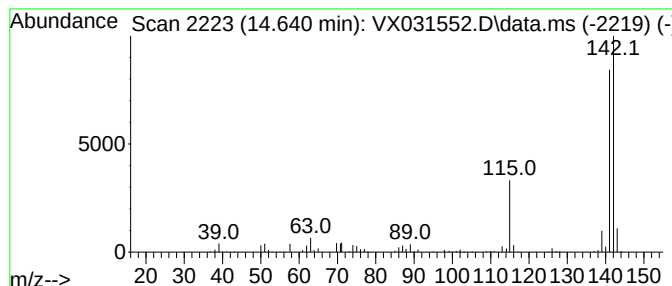
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Naphthalene, 2-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.640	26.75 ug/l	222251	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX092122\
Data File : VX031552.D
Acq On : 22 Sep 2022 06:06
Operator : JC/MD
Sample : N4642-06
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 46 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
MW-6R

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091922W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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Benzene, 1-ethy...	11.378	115.7	ug/l	961432	4	12.024	415468	50.0
Benzene, 1-ethy...	11.616	130.2	ug/l	1081670	4	12.024	415468	50.0
Benzene, 1,2,3-...	12.091	149.1	ug/l	1238900	4	12.024	415468	50.0
Indane	12.244	136.0	ug/l	1130120	4	12.024	415468	50.0
Benzene, 1-ethy...	12.616	24.1	ug/l	200541	4	12.024	415468	50.0
Benzene, 1-ethe...	12.701	38.1	ug/l	316420	4	12.024	415468	50.0
Benzene, 1,2,4,...	12.920	25.7	ug/l	213522	4	12.024	415468	50.0
Benzene, 2-ethe...	13.292	71.0	ug/l	589619	4	12.024	415468	50.0
Naphthalene, 2-...	14.640	26.8	ug/l	222251	4	12.024	415468	50.0